CLAIMS

1. A method for determining molecular shape comprising:

having a first molecule with a determined solvent-accessible molecular surface which can be visualized by a processor;

visualizing said molecular surface as a series of small area elements;

said processor performing a ray-trace, said ray-trace comprising:

starting a ray at a start point in one of said small area elements;

propagating said ray in a first direction until said ray impacts said visualized molecular surface at an impact point;

reflecting said ray from said visualized molecular surface as if said molecular surface was perfectly reflective of said ray;

recording characteristics of said ray; and

repeating said steps of starting, propagating, reflecting, and recording using the impact point of the prior iteration as the start point of the next iteration until a stop condition from a set of stop conditions is reached; and

computing a probability distribution based on characteristics of said ray, said probability distribution providing an indication of said molecule's shape.

2. The method of claim 1 wherein characteristics of said ray include at least one of: the distance of ray-trace segments and the points of impact.

3. The method of claim 2 wherein said stop condition comprises the prior recording of a predetermined number of points of impact.

4. The method of claim 3 wherein said predetermined number is 10,000.

5. The method of claim 3 wherein said predetermined number is 50,000.

6. The method of claim 3 wherein said predetermined number is 250,000.

7. The method of claim 2 wherein when said stop condition is reached, said method is repeated using at least one of a new starting point and a new direction for said ray.

8. The method of claim 1 wherein said step of recording includes recording said points of impact and determining and recording a molecular electrostatic potential (MEP) of said molecule at said points of impact.

9. The method of claim 8 wherein said probability distribution comprises an MEP-based 2D shape signature.

10. The method of claim 1 wherein said probability distribution comprises a 1D shape signature.

11. The method of claim 1 wherein said probability distribution comprises a 2D shape signature.